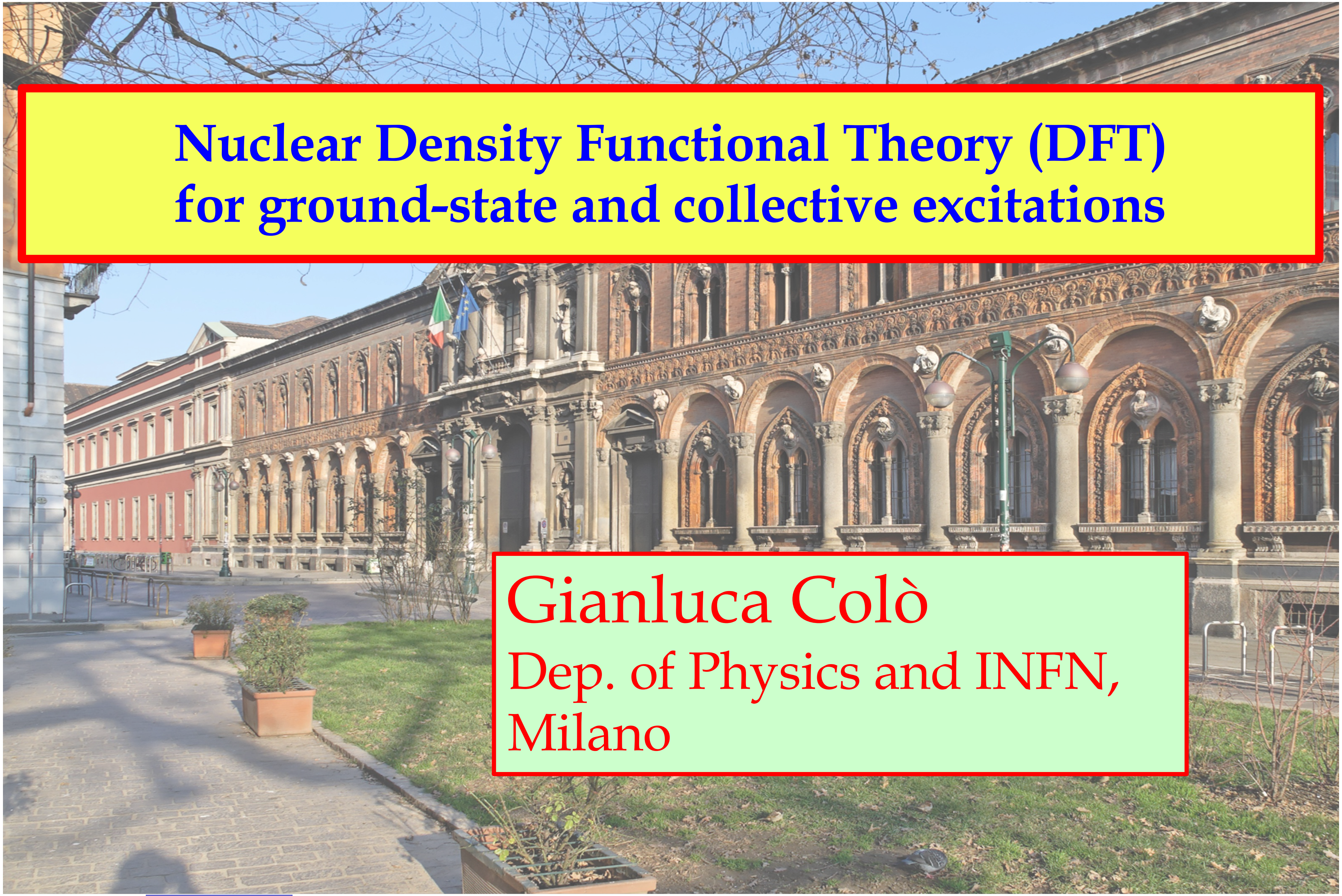

Nuclear Density Functional Theory (DFT) for ground-state and collective excitations

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ECT*, 9/7/2025

The nuclear many-body problem

There are several combinations of **nuclear Hamiltonians and many-body methods** to solve the nuclear problem.

Ab initio approaches

Configuration interaction/Shell model

Mean-field and DFT

...

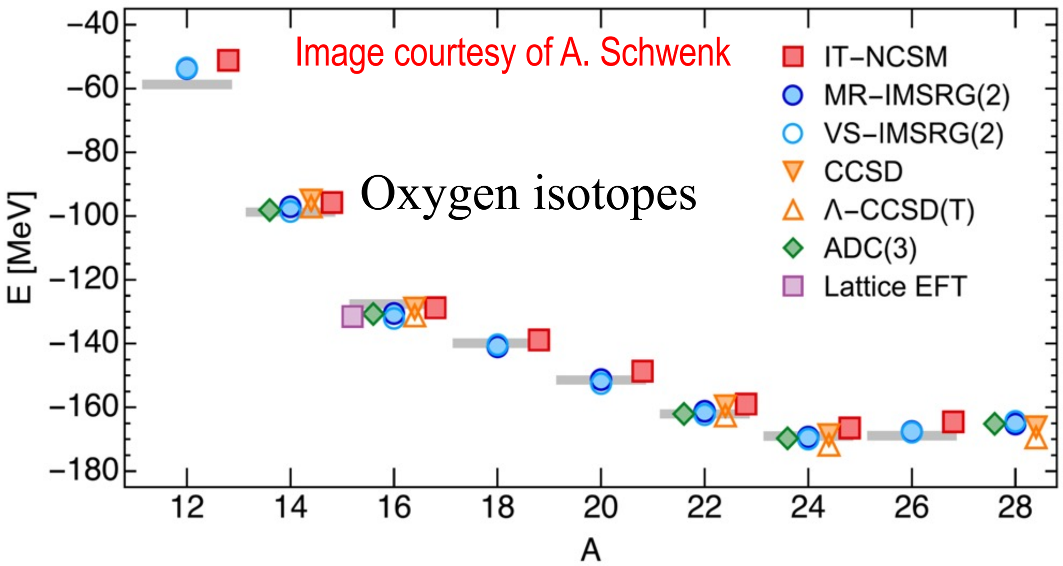
$$H\Psi = E\Psi$$

$$H = T + V = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} V_2(i,j) + \sum_{i<j<k} V_3(i,j,k)$$

Ab initio nuclear structure

Techniques to solve the many-body problem that are **exact, or systematically improvable, and can provide reliable estimates of the theoretical errors.**

Results are sensitive to the choice of the Hamiltonian.



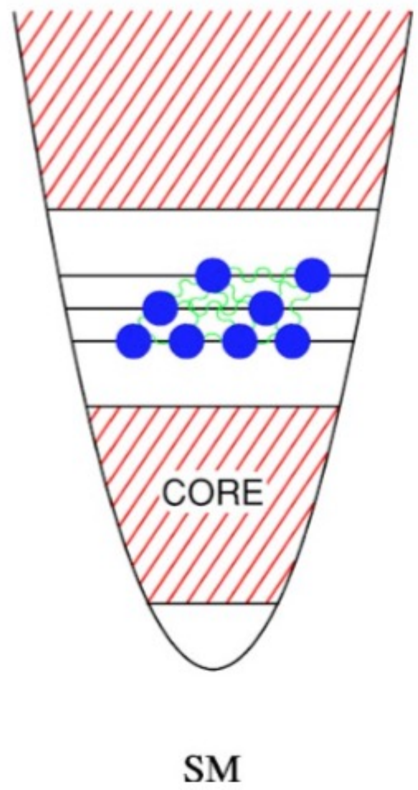
- Quantum Monte Carlo (QMC)
- Lattice EFT
- In-medium similarity renormalization group (IMSRG)
- Coupled cluster (CC)
- Self-consistent Green's function (SCGF)
- No-core Shell Model (NCSM)

...

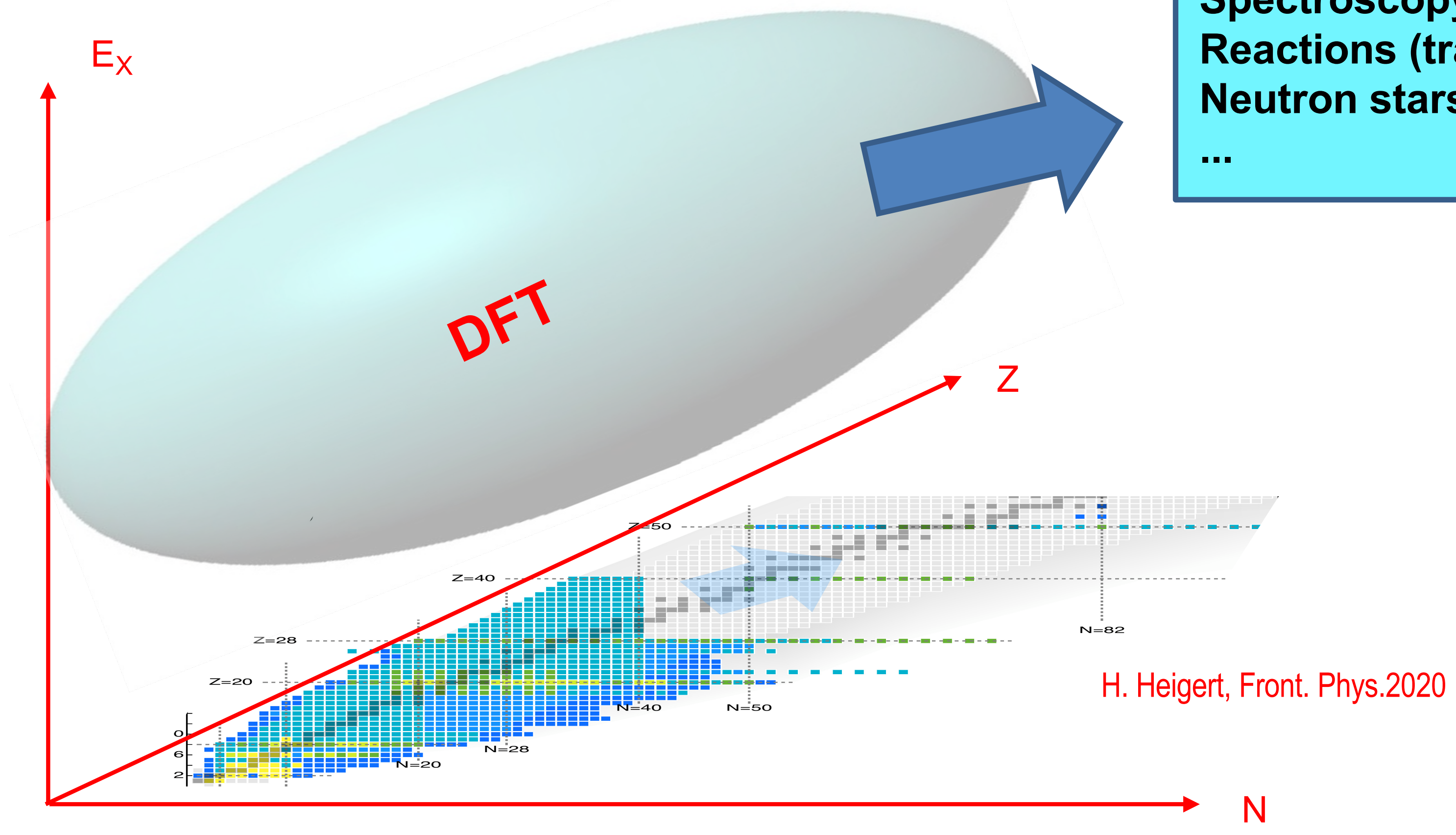
Ab initio, depending on the specific implementation, **has difficulties to handle heavy nuclei and excited states.**

Shell model or Configuration Interaction

- Nucleons (A) distributed within a given set of orbitals (n) in all possible ways.
- Roughly combinatorial, but there are ways to restrict to good J and parity.
- Diagonalization of H on this basis.
- Analogous to CI for molecules.
- Recent progress has been made concerning the SM embedded in the **continuum**.
- Role of the core...



Talk by A. GARGANO (after coffee break) !!



...
Giant Resonances and highly excited states
Spectroscopy of heavy nuclei
Reactions (transfer, fusion, fission)
Neutron stars
...

Glossary : DFT for Coulomb systems

According to Lévy and Lieb, for a system of fermions, it is possible to define an exact functional that relates energy and particle density:

$$E_{\text{exact}} = E[\rho]$$

In the case of electron systems, the **Coulomb interaction is known**. Density Functional Theory (DFT) was created initially (only) for electronic systems.

The lowest-order approximation for the energy (i.e. Hartree-Fock) is known but is not the DFT energy! There are also a few exact results for electrons.

Electronic DFT is called *ab initio*. Nonetheless, existing functionals usually include empirical parameters.

The Hohenberg-Kohn theorem

The original theorem and its proof can be found in P. Hohenberg, W. Kohn, Phys. Rev. 136, B864 (1964). They have in mind a system of interacting fermions ($H = T + V$) in some external potential V_{ext}.

a) There exist a functional of the fermion density

$$E_{V_{\text{ext}}}[\rho] = \langle \Psi | T + V + V_{\text{ext}} | \Psi \rangle = F[\rho] + \int d^3r \; V_{\text{ext}}(r)\rho(r)$$

and the part denoted by F is universal (for nuclei, it would be the only part).

b) It holds:

$$\min_\Psi \; \langle \Psi | T + V + V_{\text{ext}} | \Psi \rangle = \min_\rho \; E_{V_{\text{ext}}}[\rho]$$

The variational principle is written for the density. The w.f. may be even too large to write !! (Try as an exercise to estimate its dimension...)

The Kohn-Sham scheme

We assume that the density can be expressed in terms of **single-particle orbitals**, and that the kinetic energy has the simple form:

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r})\phi_i(\vec{r}) \qquad T = \sum_i \int d^3r\ \phi_i^*(\vec{r}) \left(-\frac{\hbar^2\nabla_i^2}{2m}\right) \phi_i(\vec{r})$$

We have said that the energy must be minimized, but we add a constraint associated with the fact that we want **orbitals that form an orthonormal set** (Lagrange multiplier):

$$E - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r}) = T + F[\rho] + \int d^3r\ V_{\rm ext}(\vec{r})\rho(\vec{r}) - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r})$$

The variation of this quantity, ($\delta/\delta\phi^*$)... = 0 produces a Schrödinger-like equation:

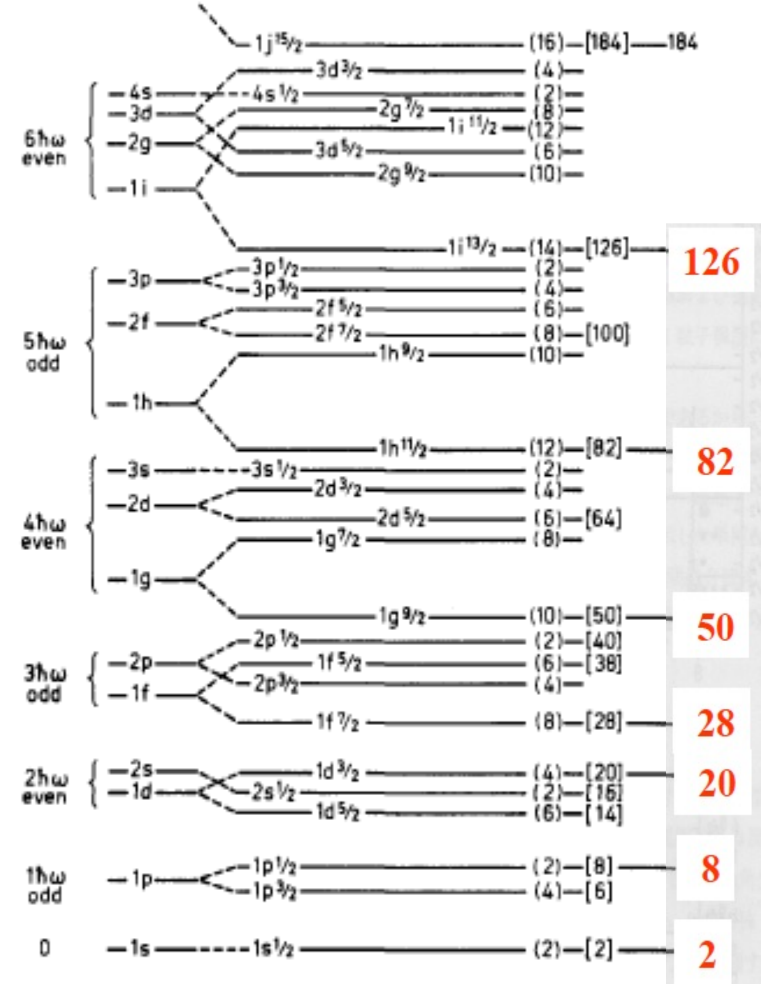
$$\left(-\frac{\hbar^2\nabla_i^2}{2m} + \frac{\delta F}{\delta\rho} + V_{\rm ext}\right)\phi_i(\vec{r}) = \varepsilon_i\phi_i(\vec{r})$$

$$h\phi_i = \varepsilon_i\phi_i$$

"DFT is an exactification of Hartree-Fock" (W. Kohn).

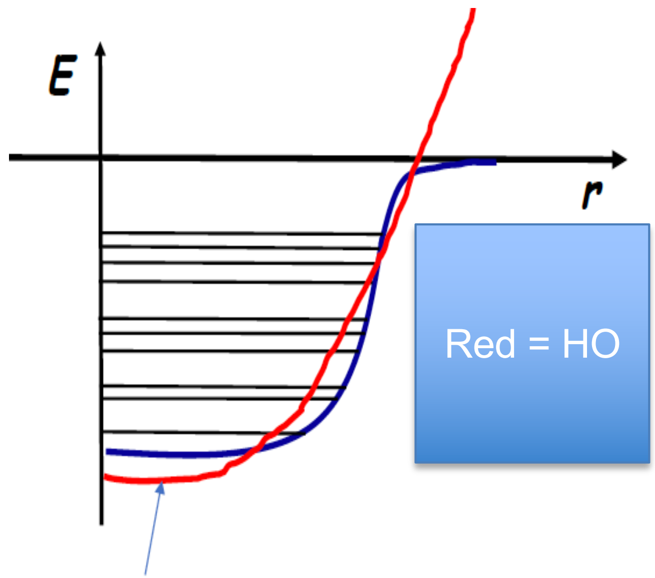
The nuclear independent particle model

≈ MeV (levels from about -50 MeV)



Many experimental evidences point to the fact that nucleons move in nuclei, to a first approximation, as **independent** particles.

Examples: evidence of shells, ground-state of nuclei around closed shells (^{17}O with Z=8, N=9 has $J^{\pi}=5/2^{+}$) …



M.G. Mayer, J.H.D. Jensen

Glossary part 2: DFT for nuclei

In the case of nuclei, we do not have (yet) a "fundamental Hamiltonian" to start from. All EDFs are based on an *ansatz* for the form of *E*, and a parameter fit.

All started with the invention of HF with effective forces. At a given point, these forces have been seen only as a way to "generate" a total energy from $\langle\Phi|T+V|\Phi\rangle$. Thus, there is no considerable difference between HF and KS-DFT.

Skyrme...

Gogny...

...and covariant EDFs

Skyrme force or "pseudo-potential"

attraction **short-range repulsion**

$$v_{\rm Skyrme} = t_0\left(1 + x_0 P_\sigma\right)\delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{2}t_1\left(1 + x_1 P_\sigma\right)\left(\vec{k}^{\dagger 2}\delta(\vec{r}_1 - \vec{r}_2) + \delta(\vec{r}_1 - \vec{r}_2)\vec{k}^2\right)$$
$$+ t_2\left(1 + x_2 P_\sigma\right)\vec{k}^\dagger \cdot \delta(\vec{r}_1 - \vec{r}_2)\vec{k} + \frac{1}{6}t_3\left(1 + x_3 P_\sigma\right)\delta(\vec{r}_1 - \vec{r}_2)\rho^\alpha\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)$$
$$+ iW_0\left(\sigma_1 + \sigma_2\right)\cdot \vec{k}^\dagger \times \delta(\vec{r}_1 - \vec{r}_2)\vec{k}$$

$$\vec{k} = -\frac{i}{2}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$

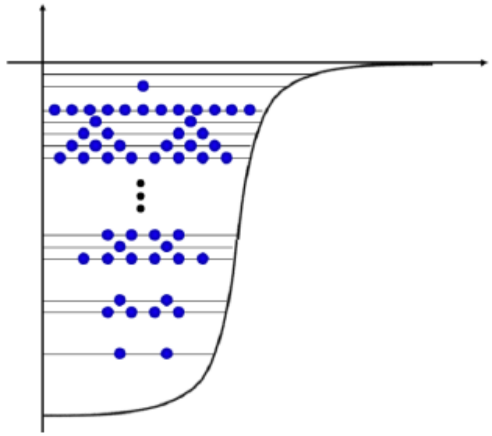
- There are velocity-dependent terms which mimic the finite-range.
- The last term is a zero-range spin-orbit.
- In total: 10 free parameters.

There are many existing Skyrme sets.
Some are available on Theo4Exp.

Total energy

E is the expectation value of H = T + v_{Skyrme} on an independent particle wave function, or Slater determinant.

$$\Phi(x_1 \ldots x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \ldots & \phi_N(x_1) \\ \ldots & \ldots & \ldots \\ \phi_1(x_N) & \ldots & \phi_N(x_N) \end{vmatrix}$$



Expectation values of 1-body and 2-body operators:

$$\langle \Phi | T | \Phi \rangle = \sum_i \langle i | t | i \rangle \qquad T = \sum_i t_i$$

$$\langle \Phi | V | \Phi \rangle = \frac{1}{2} \sum_{ij} \langle ij | v | ij \rangle_{\text{AS}} \qquad V = \sum_{ij} v(ij)$$

$$E = \int d^3r \; \mathcal{E}(\vec{r})$$

The expression for the energy can be found in P. Stevenson and M. Barton, PPNP 104, 142 (2019).

$$\begin{aligned}
\mathcal{E}(\vec{r}) = & \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left[\left(1+\frac{x_0}{2}\right)\rho^2 - \left(x_0+\frac{1}{2}\right)\sum_q \rho_q^2 + \frac{x_0}{2}\vec{s}^{\,2} - \frac{1}{2}\sum_q \vec{s}_q^{\,2}\right] \\
& + \frac{1}{12}t_3\rho^\alpha\left[\left(1+\frac{x_3}{2}\right)\rho^2 - \left(x_3+\frac{1}{2}\right)\sum_q \rho_q^2 + \frac{x_3}{2}\vec{s}^{\,2} - \frac{1}{2}\sum_q \vec{s}_q^{\,2}\right] \\
& + \left[-\frac{3t_1}{16}\left(1+\frac{x_1}{2}\right) + \frac{t_2}{16}\left(1+\frac{x_2}{2}\right)\right]\rho\nabla^2\rho + \left[\frac{3t_1}{16}\left(\frac{1}{2}+x_1\right) + \frac{t_2}{16}\left(\frac{1}{2}+x_2\right)\right]\sum_q \rho_q\nabla^2\rho_q \\
& + \left[\frac{t_1}{4}\left(1+\frac{x_1}{2}\right) + \frac{t_2}{4}\left(1+\frac{x_2}{2}\right)\right]\left(\rho\tau - \vec{j}^{\,2}\right) + \left[\frac{t_2}{4}\left(\frac{1}{2}+x_2\right) - \frac{t_1}{4}\left(\frac{1}{2}+x_1\right)\right]\sum_q\left(\rho_q\tau_q - \vec{j}_q^{\,2}\right) + \\
& + \frac{1}{8}(t_1x_1+t_2x_2)\left(\vec{s}\cdot\vec{T} - \sum_{\alpha\beta}\mathbf{J}_{\alpha\beta}\mathbf{J}_{\alpha\beta}\right) - \frac{1}{32}(3t_1x_1 - t_2x_2)\,\vec{s}\cdot\nabla^2\vec{s} + \\
& \frac{1}{8}(t_2-t_1)\sum_q\left(\vec{s}_q\cdot\vec{T}_q - \sum_{\alpha\beta}\mathbf{J}_{q,\alpha\beta}\mathbf{J}_{q,\alpha\beta}\right) + \frac{1}{32}(3t_1+t_2)\,\vec{s}_q\cdot\nabla^2\vec{s}_q \\
& - \frac{1}{2}W_0\sum_{qq'}(1+\delta_{qq'})\left(\vec{s}_q\cdot\vec{\nabla}\times\vec{j}_{q'} + \rho_q\vec{\nabla}\cdot\vec{J}_{q'}\right)
\end{aligned}$$

The expression is complicated because different kinds of densities appear...

However, the expression simplifies in even-even nuclei. Our code(s) are for spherical, even-even nuclei

From the total energy to HF equations

The total energy is written in terms of densities; and, in turn, the densities are written in terms of s.p. wave functions or orbitals.

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r})\phi_i(\vec{r})$$

$$\delta \left[E - \sum_i \varepsilon_i \int d^3r \ \phi_i^*(\vec{r})\phi_i(\vec{r}) \right]$$

This variation leads to HF (or HF-like) equations

$$\left[-\vec{\nabla} \frac{\hbar^2}{2m_q^*(\vec{r})} \cdot \vec{\nabla} + U_q(\vec{r}) + \delta_{q,p} U_{\rm Coul}(\vec{r}) - i\vec{W}_q(\vec{r}) \cdot \left(\vec{\nabla} \times \vec{\sigma} \right) \right] \phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r})$$

Our code solves these equations in **spherical symmetry**, and on a radial mesh.
The method is **iterative** and, at convergence, the s.p. energies are stable while the energy reaches its MINIMUM.

Results

See the talk by Imane Moumene (after the coffee break).

Total energy and breakdown of different contributions, single-particle energies and wave functions, densities and some of their moments like <r^2>.

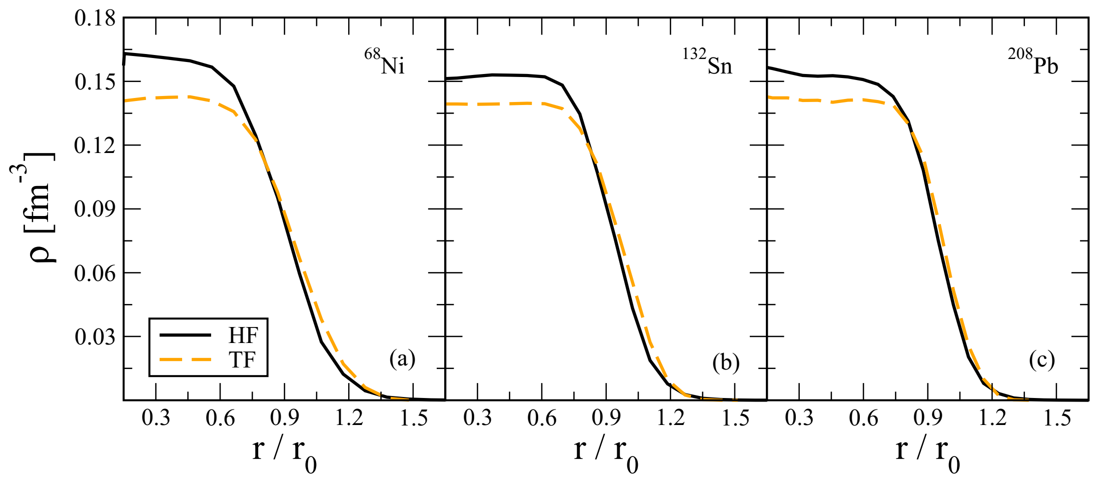
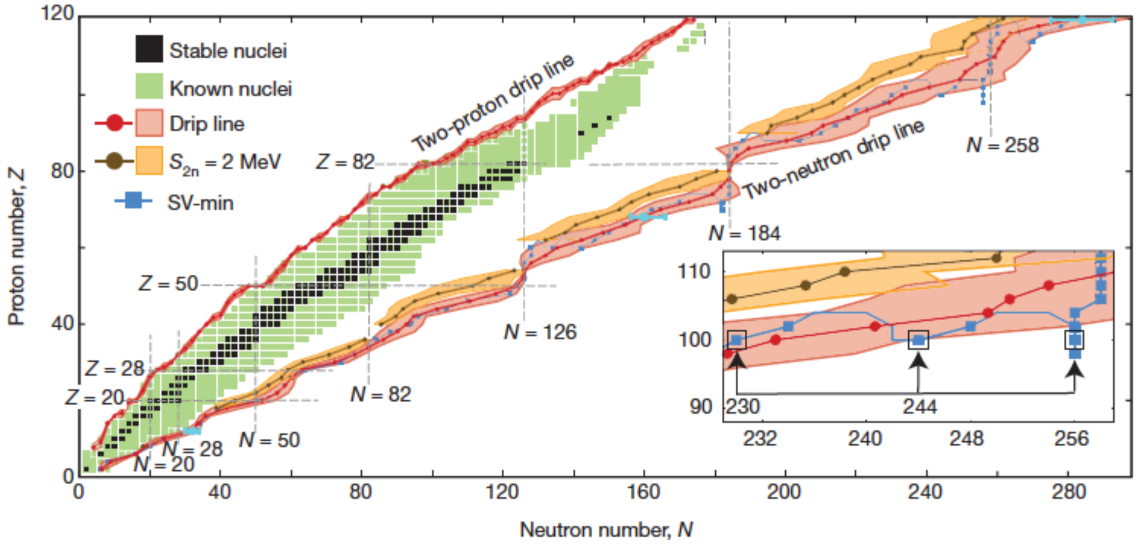


FIG. 1. The isoscalar density profiles for ^{68}Ni, ^{132}Sn, and ^{208}Pb, from Hartree-Fock and Thomas-Fermi models, versus the normalized radius r/r_0, with $r_0 = 1.2A^{1/3}$.

The drip lines

J. Erler *et al.*, Nature 486, 509 (2012) - SEDF



A.V. Afanasjev *et al.*, Phys. Lett. B726, 680 (2013) - CEDF

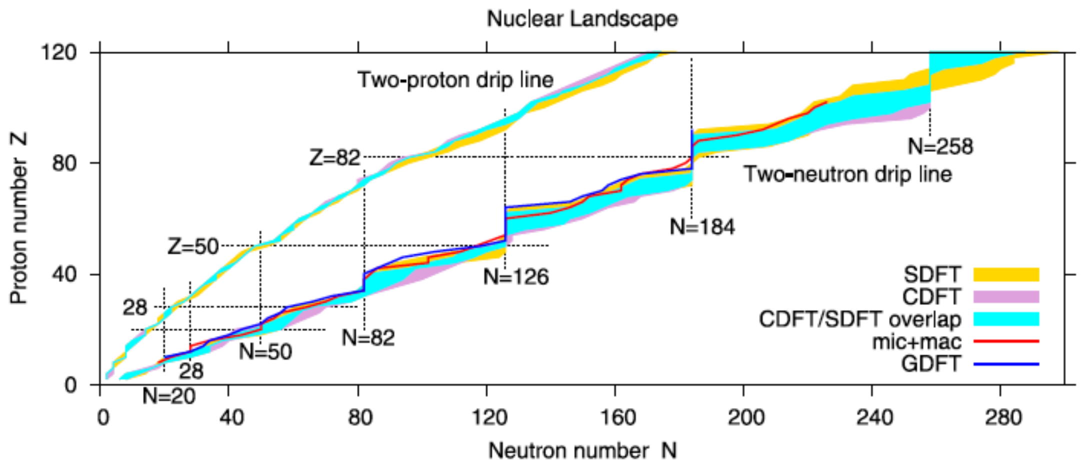


Fig. 4. The comparison of the uncertainties in the definition of two-proton and two-neutron drip lines obtained in CDFT and SDFT. The shaded areas are defined by the extremes of the predictions of the corresponding drip lines obtained with different parametrizations. The blue shaded area shows the area where the CDFT and SDFT results overlap. Non-overlapping regions are shown by dark yellow and plum colors for SDFT and CDFT, respectively. The results of the SDFT calculations are taken from the supplement to Ref. [2]. The two-neutron drip lines obtained by microscopic + macroscopic (FRDM [3]) and Gogny D1S DFT [5] calculations are shown by red and blue lines, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this Letter.)

Nuclear collective vibrations

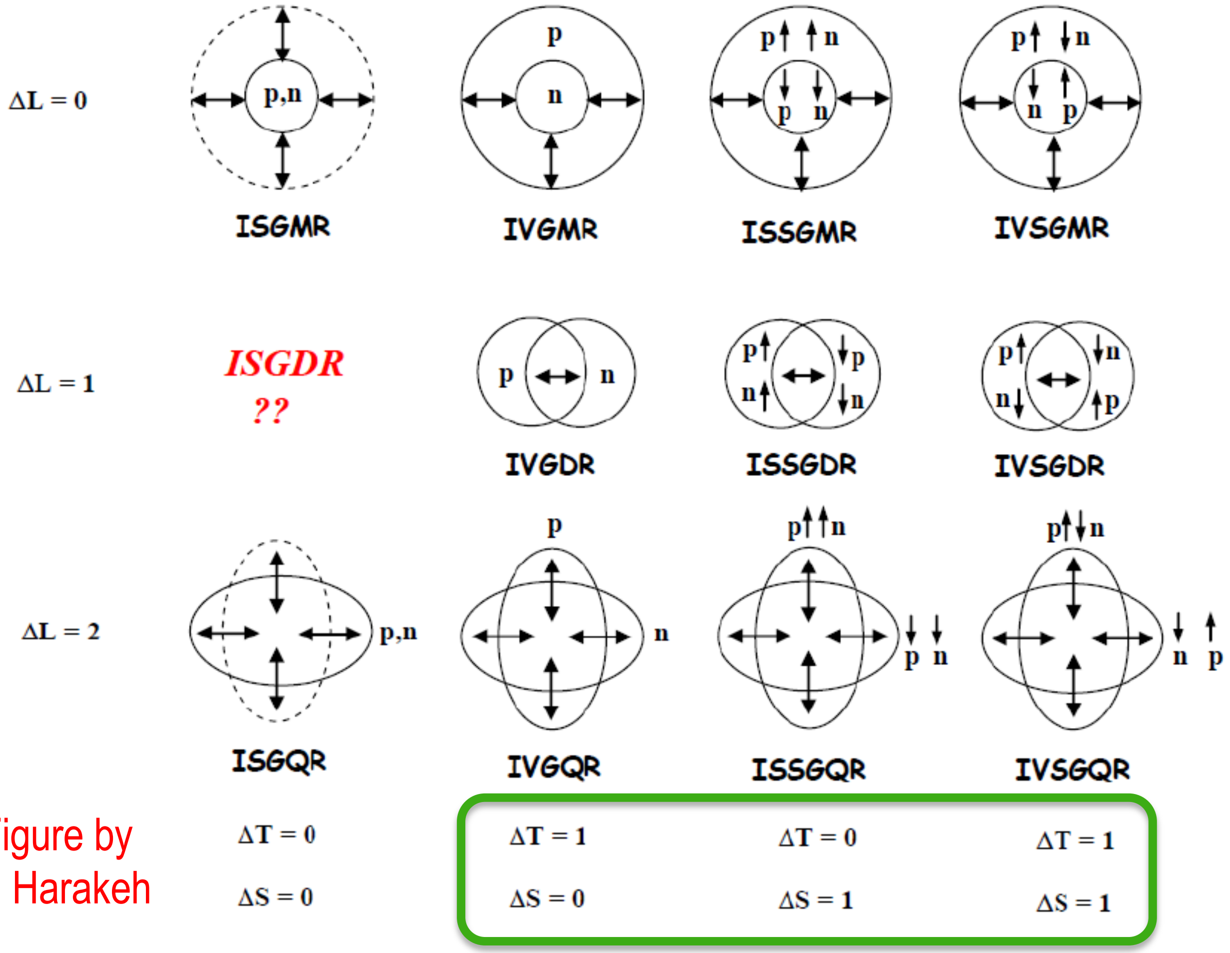


Figure by
M. Harakeh

IS = Iso-Scalar
IV = Iso-Vector
S = Spin
G = Giant
M = Monopole
D = Dipole
Q = Quadrupole
O = Octupole

Strength function and operators

$$S(E) = \sum_n |\langle n|F|0\rangle|^2 \, \delta\left(E - E_n\right)$$

$$S(E) = \sum_n |\langle n|F|0\rangle|^2 \frac{\Gamma_n}{(E - E_n)^2 + \frac{\Gamma_n^2}{4}}$$

Isoscalar (T=0) vs. isovector (T=1) and electric (S=0) vs. magnetic (S=1) operators.

$$F_{\rm IS} = \sum_i r_i^L Y_{LM}(\hat{r}_i),$$

$$F_{\rm IV} = \sum_i r_i^L Y_{LM}(\hat{r}_i)\tau_z(i).$$

$$F_{\rm IS} = \sum_i r_i^L \left[Y_{LM}(\hat{r}_i) \otimes \boldsymbol{\sigma}(i)\right]_J,$$

$$F_{\rm IV} = \sum_i r_i^L \left[Y_{LM}(\hat{r}_i) \otimes \boldsymbol{\sigma}(i)\right]_J \tau_z(i).$$

$$F_{\rm ISGMR} = \sum_i r_i^2,$$

$$F_{\rm IVGMR} = \sum_i r_i^2 \tau_z(i).$$

$$F_{\rm IVGDR} = \frac{eN}{A}\sum_{i=1}^{Z} r_i Y_{1M}(\hat{r}_i) - \frac{eZ}{A}\sum_{i=1}^{N} r_i Y_{1M}(\hat{r}_i).$$

C.o.m. subtracted

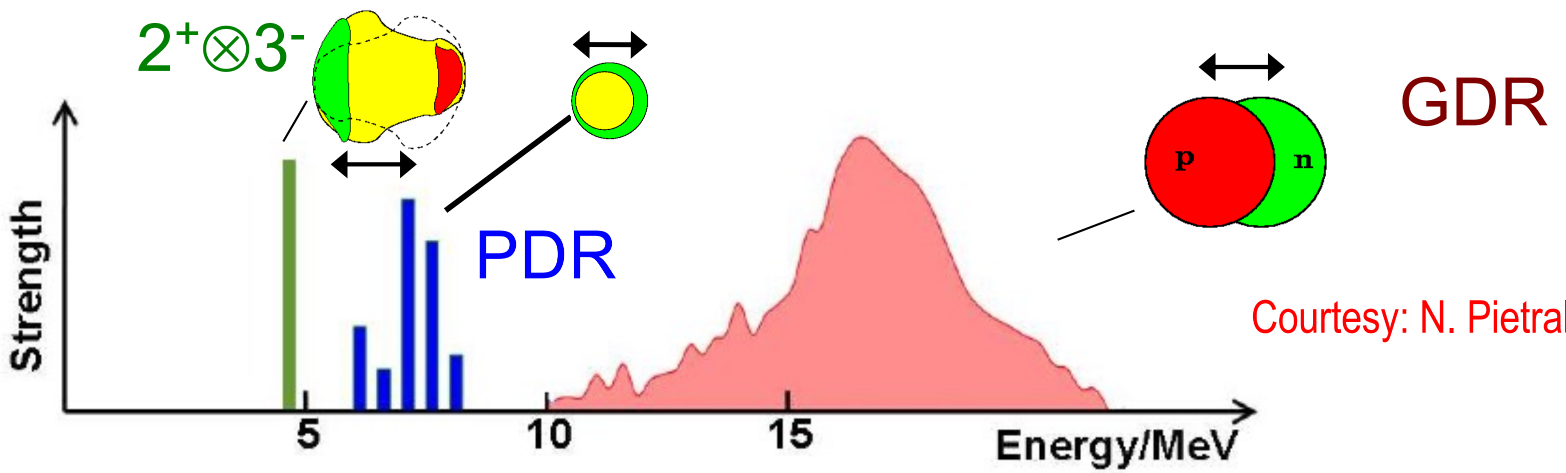
Collectivity

Given the strength function, one can define its moments:

$$m_0 \equiv \int dE \; S(E)$$ Total strength

$$m_1 \equiv \int dE \; E \; S(E)$$ EWSR

Often, some states exhaust most of the total strength of or the EWSR.

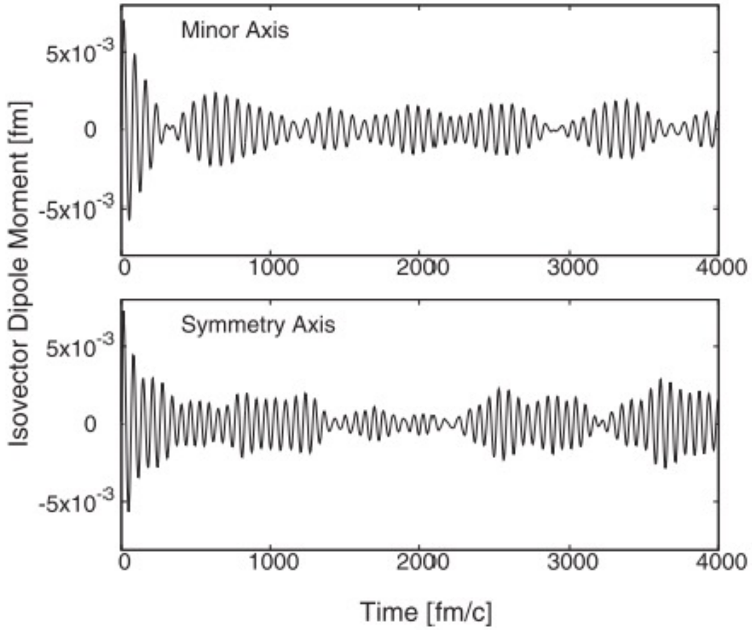


Courtesy: N. Pietralla

Time-dependent Hartree-Fock or Kohn-Sham

$$h\phi_i = \varepsilon_i \phi_i$$

From: P. Stevenson (U. Surrey)



In the time-dependent case, one can solve the **evolution equation for the density** directly:

$$h(t) = h + f(t) \qquad [h(t), \rho(t)] = i\hbar\, \dot{\rho}(t)$$

$$\rho(t=0) \neq \rho_{\rm g.s.}$$

$$\rho(t=\Delta t) = U(t=0, t=\Delta t)\rho(t=0) \qquad U = e^{-i\frac{\Delta t}{\hbar}\cdot h}$$

This approach allows also studying large-amplitude motion (e.g. reactions).

If the equation for the density is **linearized** (small amplitude limit or linear response): **Random Phase Approximation or RPA**.

Matrix RPA and Finite Amplitude Method (FAM)

$$\rho = \rho^{(0)} + \delta\rho \qquad h = h^{(0)} + \delta h$$

Small amplitude
Harmonic approx.

$$\delta\rho = \delta\rho(\vec{r})\mathrm{e}^{-i\omega t} + \mathrm{h.c.}$$

$$\hbar\omega\delta\rho(\omega) = \left[h^{(0)}, \delta\rho(\omega)\right] + \left[\delta h(\omega), \rho^{(0)}\right] + \left[f, \rho^{(0)}\right]$$

Standard definition of the "forward" and "backward" amplitudes:

$$X_{\mathrm{ph}} = \langle \mathrm{ph}^{-1} | \delta\rho | 0 \rangle \qquad Y_{\mathrm{ph}} = \langle \mathrm{hp}^{-1} | \delta\rho | 0 \rangle$$

$$(\varepsilon_p - \varepsilon_h - \omega)\, X_{\mathrm{ph}} + \delta h^{\mathrm{ph}}(\omega) = -f^{\mathrm{ph}}(\omega)$$
$$(\varepsilon_p - \varepsilon_h + \omega)\, Y_{\mathrm{ph}} + \delta h^{\mathrm{hp}}(\omega) = -f^{\mathrm{hp}}(\omega)$$

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar\omega \begin{pmatrix} X \\ Y \end{pmatrix}$$

FAM: the calculation of the two-body matrix elements is avoided

Matrix formulation

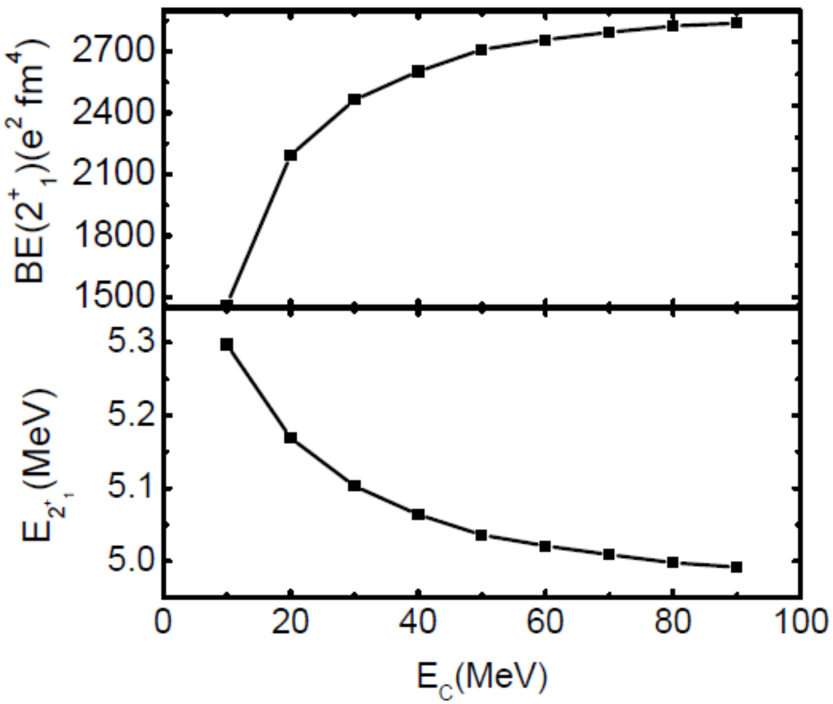
$$\delta h = \sum \frac{\delta h}{\delta \rho} \delta\rho$$

G.C. et al., Computer Physics Commun. 184, 142 (2013).

The RPA program

The continuum is discretized. The basis must be large due to the zero-range character of the force. Parameters: R, E_C.

^{208}Pb - SGII



One possible issue:
Since the code is spherical, it may be prone to **instabilities** when calculating e.g. 2^+ states in a nucleus which is actually deformed.
Signal: imaginary solution.

Cf. Imane's talk for more details and examples.

RPA and collectivity: schematic model (I)

Schematic 2 x 2 case

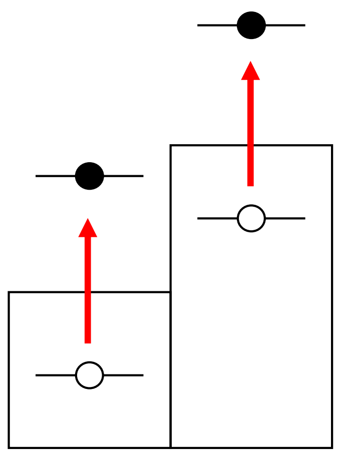
$$\begin{pmatrix} \varepsilon + v & v \\ v & \varepsilon + v \end{pmatrix}$$

$$\hbar\omega_1 = \varepsilon, \qquad X^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

$$\hbar\omega_2 = \varepsilon + v \qquad X^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Magnetic spin-flip states (M1)

^{208}Pb : $h_{11/2} \rightarrow h_{9/2}$ (proton)
$i_{13/2} \rightarrow i_{11/2}$ (neutron)

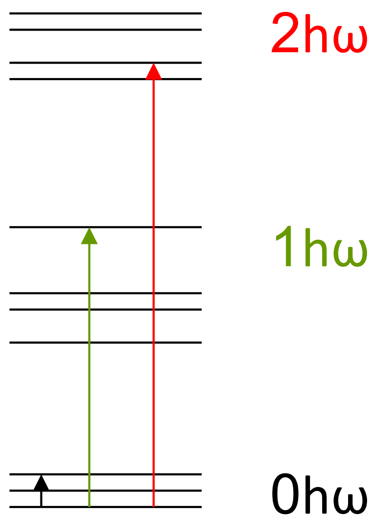


RPA and collectivity: schematic model (II)

Schematic *N* x *N* case

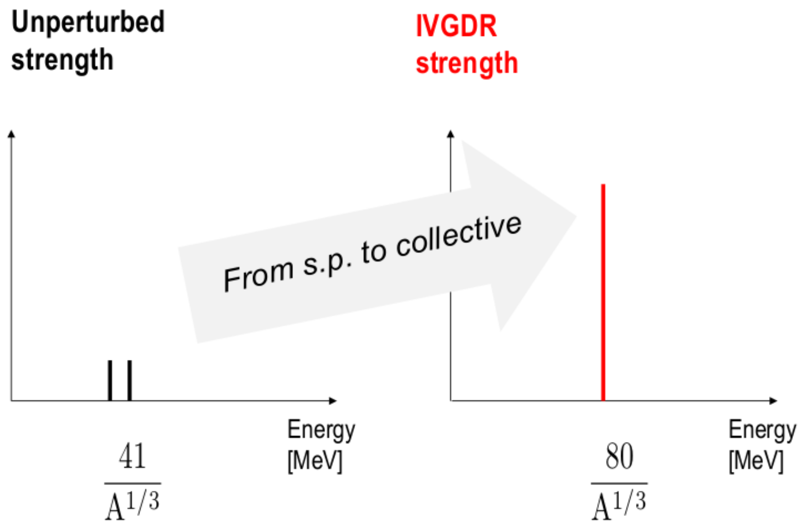
There is one “coherent state”:

$$\frac{1}{\sqrt{N}}\begin{pmatrix} 1 \\ 1 \\ \dots \\ 1 \end{pmatrix}$$



Its transition amplitude is enhanced:

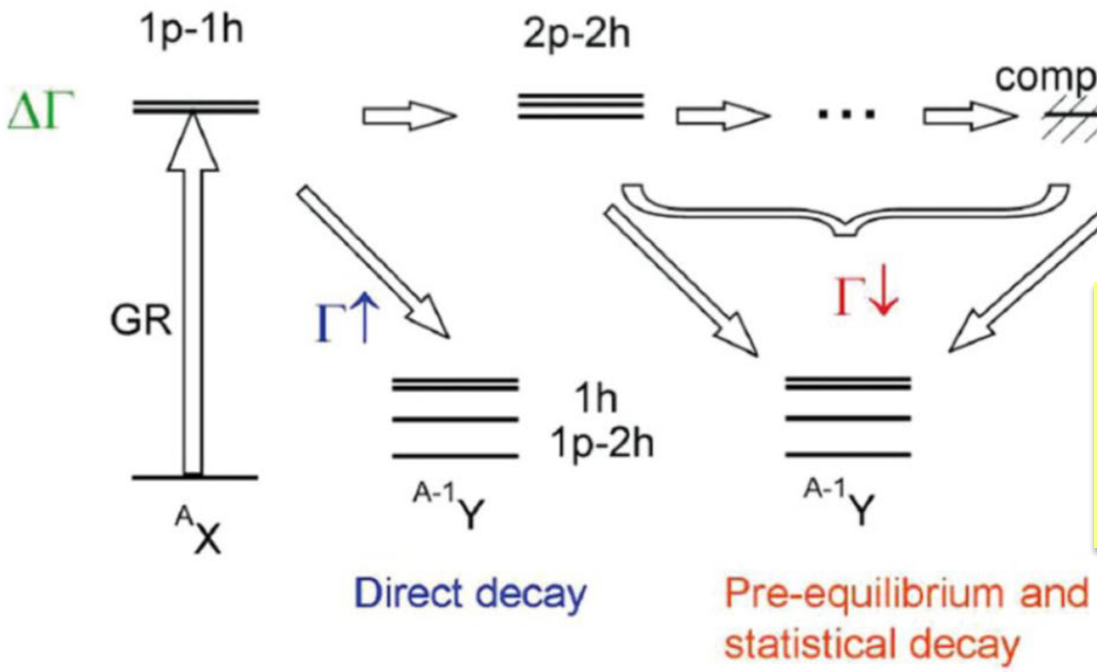
$$\langle n|F|0\rangle = \sum_{ph} X_{ph}\langle p|F|h\rangle \approx N\frac{1}{\sqrt{N}}M = \sqrt{N}\ M$$



G. C., *Theoretical Methods for Giant Resonances*, in: Handbook of Nuclear Physics, edited by I. Tanihata, H. Toki and T. Kajino (Springer, 2022).

Giant resonances are **NOT** sharp states but have a large width (several MeV)

$$\Gamma = \underbrace{\Gamma_{\text{Landau}} + \Gamma^{\downarrow}}_{\text{Internal mixing}} + \underbrace{\Gamma^{\uparrow} + \Gamma_{\gamma}}_{\text{Decay}}$$

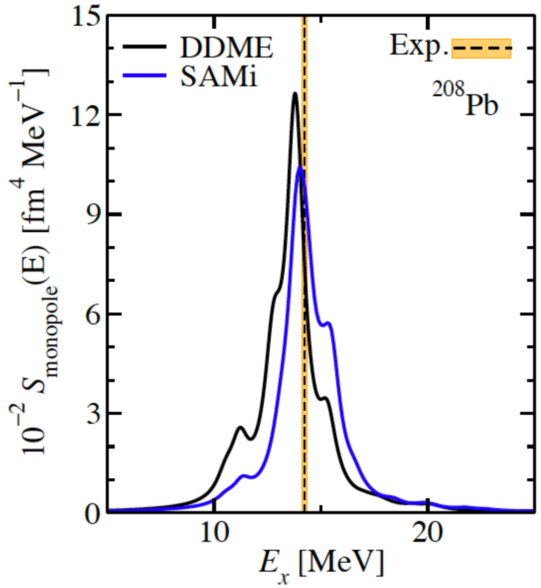


If this picture clear in all details? We do not have systematic data and full understanding (cf. also β-delayed neutron emission).

This is a **challenge for theory** and may not simply call for parameter tuning but is related to fundamental questions (many-body theory, open quantum systems, the concept of thermalization...).

Giant Monopole Resonance

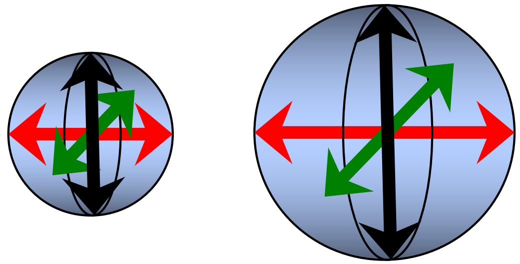
Example of study which is not carried out for mere “academic purposes”, but to shed light on **more general properties of nature**…



SN1987a

Breathing mode: in this case its energy is correlated with the compressibility of nuclear matter.

$$\chi \equiv -\frac{1}{\Omega}\left(\frac{\partial P}{\partial \Omega}\right)^{-1}$$



We better consider the density as a variable. $\rho = \frac{A}{\Omega}$

Incompressibility: $$\chi^{-1} = \rho^3 \frac{d^2}{d\rho^2}\left(\frac{E}{A}\right)$$

$$K_\infty = 9\rho_0^2 \frac{d^2}{d\rho^2}\left(\frac{E}{A}\right)_{\rho=\rho_0}$$

(**around 240 MeV**)

U. Garg, GC, PPNP 101 (2018) 55

All this did not consider pairing, namely it was supposed to work for magic nuclei...

...we move to the superfluid case

Exercise 1

^{16}O RPA 3^- SLy5 default parameters

	E	B(IS)	%M0(IS)	B(EM)	B(IV)	%M0(IV)
1	0.67601E+01	0.25645E+04	0.21411E+02	0.68716E+03	0.31934E+01	0.37180E-01

E_{exp}
6.13 MeV

^{20}O RPA 2^+ SLy5 default parameters: instability!

^{20}O QRPA 2^+ SLy5 box = 16 fm, E_{max} = 60 MeV:

	E	BEL_is	FRAC_NEWSR	BEL_em	BEL_iv	FRAC_NEWSR
1	0.20563E+01	0.37183E+03	0.37028E+02	0.12147E+02	0.15160E+03	0.23528E+02

Exercise 2

^{A}O : A=16-24

SLy5. Box size = 15 fm

A	E	E_{exp}	$<r_p>^{1/2}$	$<r_p>^{1/2}_{exp}$	$<r_n>^{1/2}$	Δ_n
16	128.40	127.52	2.68	2.59	2.66	0
18	141.18	139.81	2.69	2.68	2.83	1.19
20	153.36	151.40	2.70		2.96	1.29
22	163.30	162.00	2.71		3.06	0.76
24	171.30	168.90	2.74		3.20	0

Exp. energies from `nndc.bnl.gov`; exp. proton radii from De Vries *et al.*, ATNDT 36, 495 (1987).

Exercise 3

Hot pygmy dipole strength in nickel isotopes

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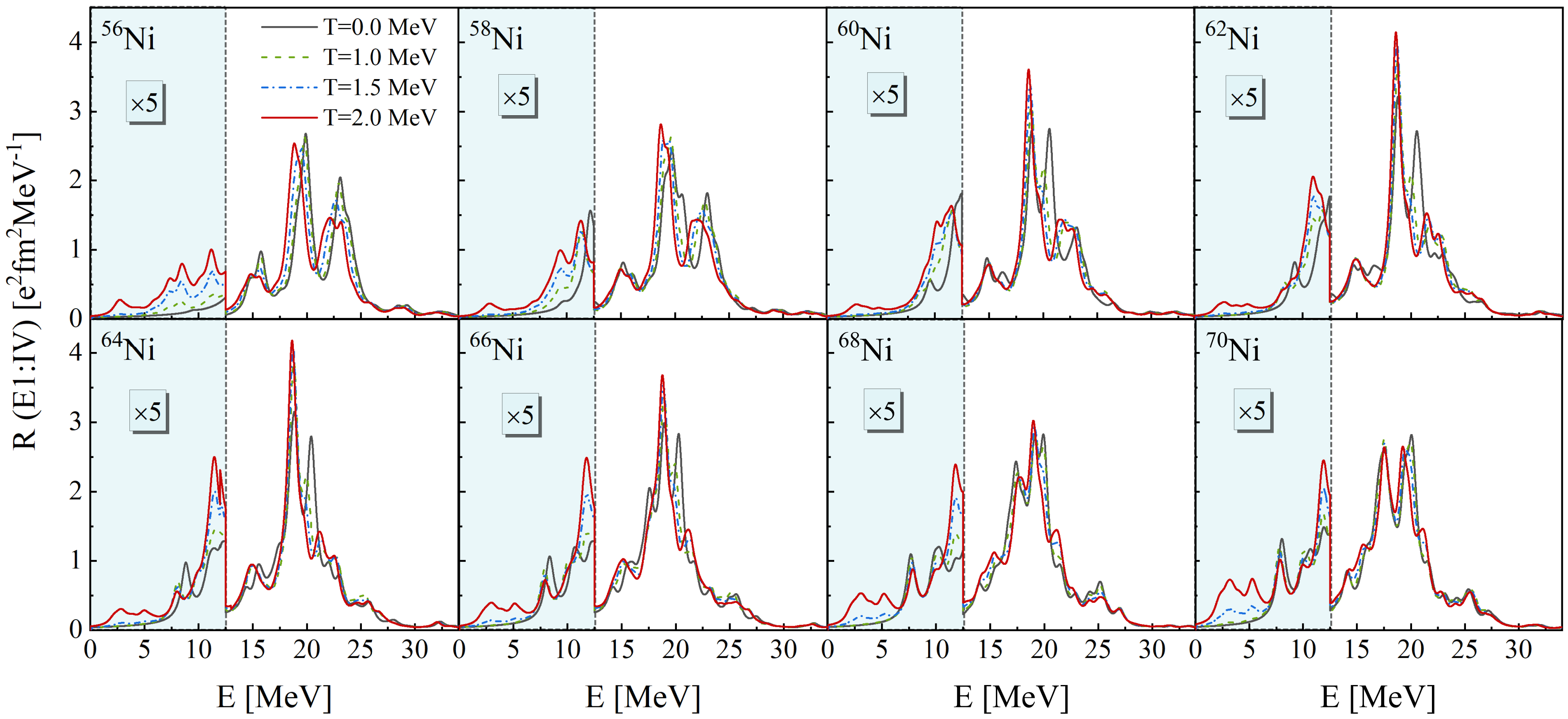
(Dated: June 17, 2025)



arXiv:2506.13354v1

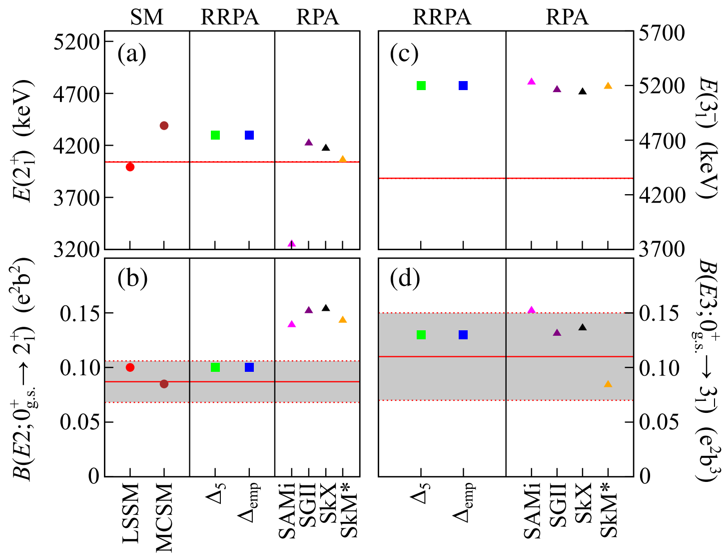
RPA and the nuclear Shell Model (SM)

PHYSICAL REVIEW LETTERS **121,** 252501 (2018)

Enhanced Quadrupole and Octupole Strength in Doubly Magic ^{132}Sn

D. Rosiak,[1] M. Seidlitz,[1,*] P. Reiter,[1] H. Naïdja,[2,3,4] Y. Tsunoda,[5] T. Togashi,[5] F. Nowacki,[2,3] T. Otsuka,[6,5,7,8,9] G. Colò,[10,11] K. Arnswald,[1] T. Berry,[12] A. Blazhev,[1] M. J. G. Borge,[13,†] J. Cederkäll,[14] D. M. Cox,[15,16] H. De Witte,[8] L. P. Gaffney,[13] C. Henrich,[17] R. Hirsch,[1] M. Huyse,[8] A. Illana,[8] K. Johnston,[13] L. Kaya,[1] Th. Kröll,[17] M. L. Lozano Benito,[13] J. Ojala,[15,16] J. Pakarinen,[15,16] M. Queiser,[1] G. Rainovski,[18] J. A. Rodriguez,[13] B. Siebeck,[1] E. Siesling,[13] J. Snäll,[14] P. Van Duppen,[8] A. Vogt,[1] M. von Schmid,[17] N. Warr,[1] F. Wenander,[13] and K. O. Zell[1]

(MINIBALL and HIE-ISOLDE Collaborations)



theory [11,12]. Because of the computational limits of the valence space, the SM approaches do not provide information on the 3^-_1 state. The RPA and RRPA calculations

In addition, the shell model cannot provide response at high energy (cross sections for high-E neutrinos, just to make an example, are doable within RPA and QRPA but not SM).

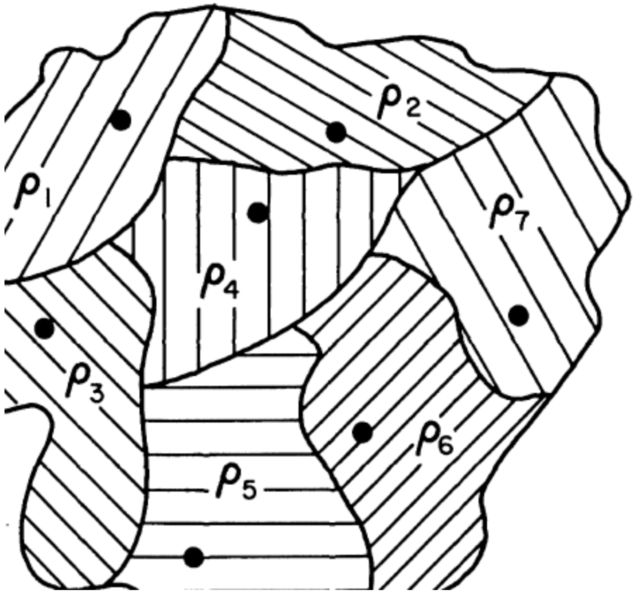
Backup slides

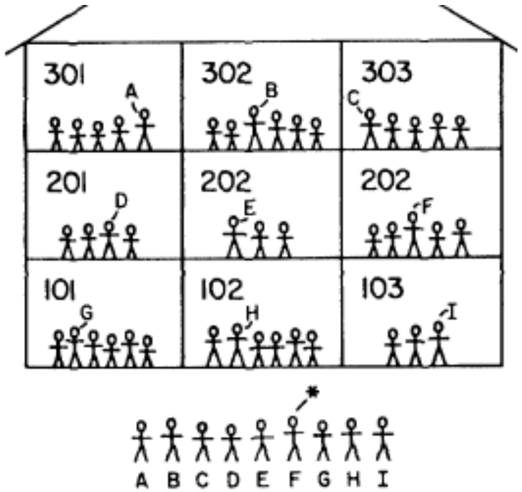
The constrained search approach by Lévy-Lieb

$$E_0 = \min_\Psi \langle \Psi | H | \Psi \rangle,$$

$$E_0 = \min_\rho \left(\min_{\Psi \to \rho} \langle \Psi | H | \Psi \rangle \right) = \min_\rho E[\rho],$$

$$\boxed{E[\rho] = \min_{\Psi \to \rho} \langle \Psi | H | \Psi \rangle.}$$





We consider all w.f.'s that correspond to a specific density with the symbol

$$\Psi \to \rho$$

"instead of finding the tallest child in the school by lining all of them in the yard, we just line in the yard the tallest pupils of each class..."

Note on exchange operators

The operator

$$P_{12} \equiv P_M P_\sigma P_\tau$$

exchanges particles 1 and 2 (position, spin and isospin are exchanged, respectively, by the three operators at r.h.s.).
It is useful because one can write

$$\langle ij|V|kl\rangle_{\mathrm{AS}} = \langle ij|V\,(1 - P_{12})\,|kl\rangle.$$

In the case of a zero-range force P_M=number:
1 for $V = a\delta(\vec{r}_{12})$. ($\vec{r}_{12} \equiv \vec{r}_1 - \vec{r}_2$).

$$P_\sigma = \frac{1 + \sigma_1\sigma_2}{2}.$$

Fitting the EDF parameters

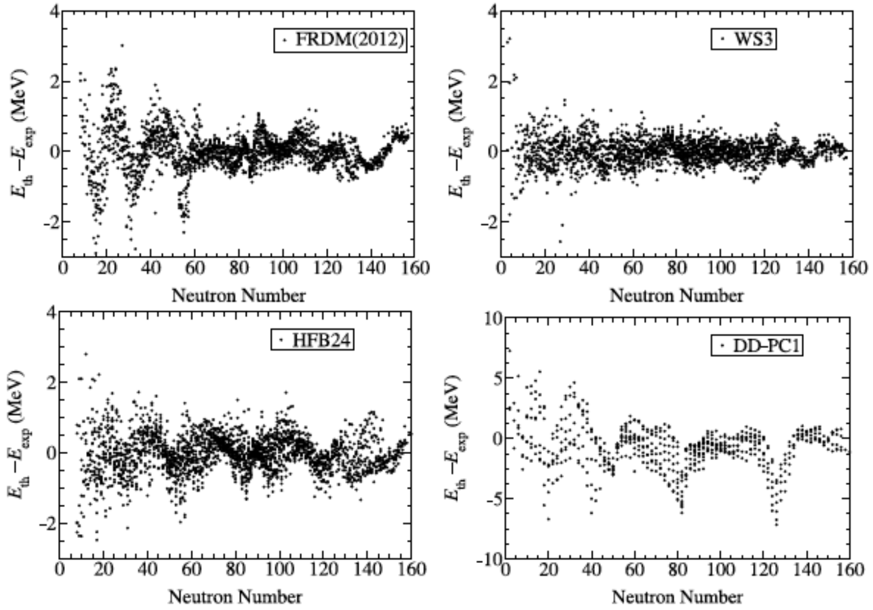
- Empirical saturation point
- Masses of nuclei
- Charge radii of nuclei
- More pseudo-observables like the equation of state of neutron matter
- More observables: excited states
- *A bit outside DFT philosophy: single-particle states and spin-orbit splittings*

$$\chi^2(\vec{p}\,) = \sum_{k=1}^{N_{\rm data}} \frac{\left(O_k^{\rm th.}(\vec{p}\,) - O_k^{\rm exp.}\right)^2}{(\Delta O)^2}$$

χ-square fitting is one widely used option to obtain the EDF parameters

Increasing number of studies that employ Bayesian techniques (parameter distributions)

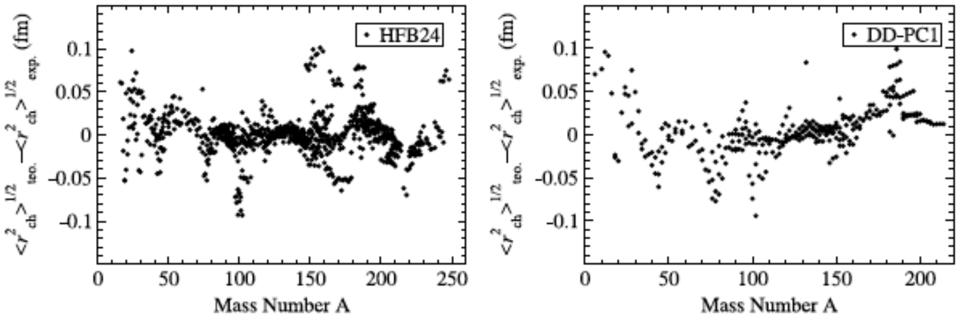
Masses and charge radii of atomic nuclei

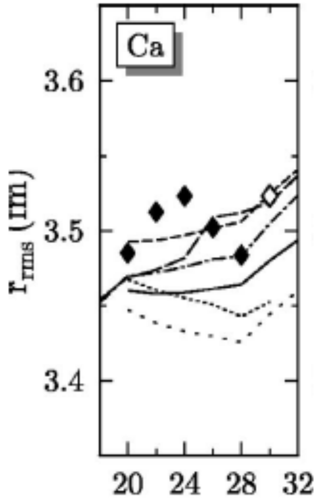


Model	Type	N° par.	σ_M [MeV]
FRDM(2012)	Mac-Mic	38[a]	0,559[b]
WS4[c]	Mac-Mic	18	0,298[d]
HFB24	EDF	30[e]	0,549[f]
UNEDF1	EDF	12	1,88[g]
DD-PC1	EDF	9	2,01[h]

Masses: typical errors ≈ MeV. "Arches" show up.

X. Roca-Maza and N. Paar, PPNP 101, 96 (2018)





From M. Bender

For radii the pictures is somehow more blurred. More fingerprints of the basic limitations of the current EDFs.

RPA and TDHF

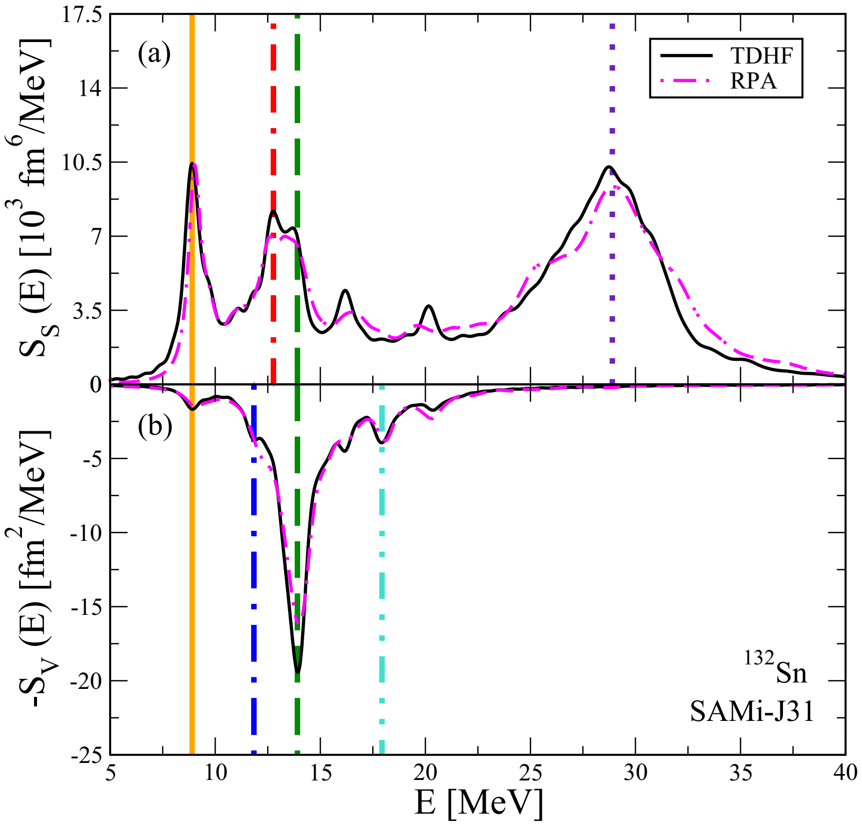


FIG. 9. The strength function of the IS (a) and IV (b) response for ^{132}Sn with SAMi-J31 as obtained in TDHF or in RPA calculation, with $L_{\text{box}} = 20$ or 30 fm, respectively. The vertical lines indicate the energy of the modes selected for the transition density analysis (see Sec. III E).

This comparison between TDHF and RPA (using Skyrme EDFs) is taken from:

S. Burrello *et al.*, Phys. Rev. C99, 054314 (2019).

The nuclear EoS and the symmetry energy (I)

- From the energy per particle as a function of the density we can extract the pressure.

$$P(\rho) = \rho^2 \frac{\partial}{\partial \rho} \frac{E}{A}(\rho)$$

- For this reason, we call E/A the “equation of state” of nuclear matter.

- In this quantity, the part that depends on the neutron-proton imbalance is poorly known.

Nuclear matter EOS

Symmetric matter EOS

Symmetry energy S

$$\frac{E}{A}(\rho, \beta) = \frac{E}{A}(\rho, \beta = 0) + S(\rho)\beta^2$$

$$\beta \equiv \frac{\rho_n - \rho_p}{\rho}$$

- Odd powers forbidden by isospin symmetry
- Up to densities relevant for nuclear physics this “quadratic approximation” seems to hold

The nuclear EoS and the symmetry energy (II)

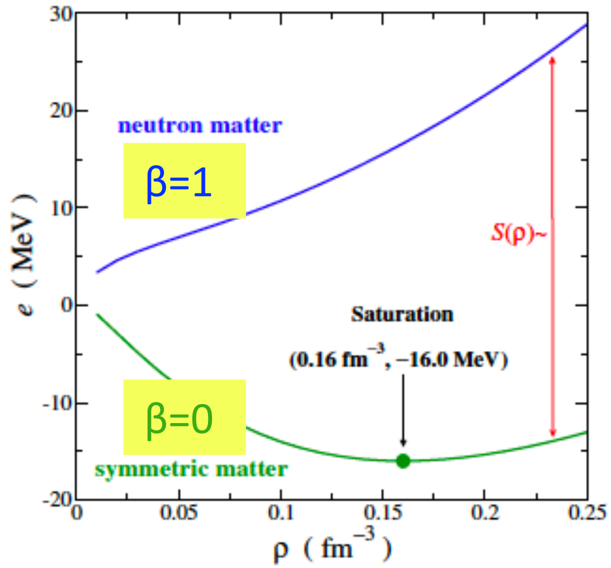
Nuclear matter EOS

Symmetric matter EOS

Symmetry energy S

$$\frac{E}{A}(\rho,\beta) = \frac{E}{A}(\rho,\beta=0) + S(\rho)\beta^2$$

$$\beta \equiv \frac{\rho_n - \rho_p}{\rho}$$



$$S \equiv \frac{E}{A}(\text{neutron matter}) - \frac{E}{A}(\text{symmetric matter})$$

In turn, the symmetry energy can be expanded around a reference density.
One usually takes the saturation energy of symmetric matter:

$$\rho_0 = 0.16\ \text{fm}^{-3}$$

The nuclear EoS and the symmetry energy (III)

Expansions around ρ_0= 0.16 fm^{-3} SATURATION POINT of SNM

$$\frac{E}{A}(\rho,\beta=0) = E_0 + \frac{1}{2}K_\infty\left(\frac{\rho-\rho_0}{3\rho_0}\right)^2 + \ldots$$

$$S(\rho) = J + L\left(\frac{\rho-\rho_0}{3\rho_0}\right) + \frac{1}{2}K_{\rm sym}\left(\frac{\rho-\rho_0}{\rho_0}\right)^2 + \ldots$$

$$S(\rho_0) \equiv J$$
$$S'(\rho_0) \equiv L/3\rho_0$$
$$S''(\rho_0) \equiv K_{\rm sym}/9\rho_0^2$$

$J = S_0 = S_v = a_4 = a_\tau$

J.M. Lattimer, Y. Lim, Astr. J. **771,** 51 (2013)

B.A. Li and X. Han, PLB **727**, 276 (2013)

M. Oertel *et al.*, RMP **89**, 015007 (2017)

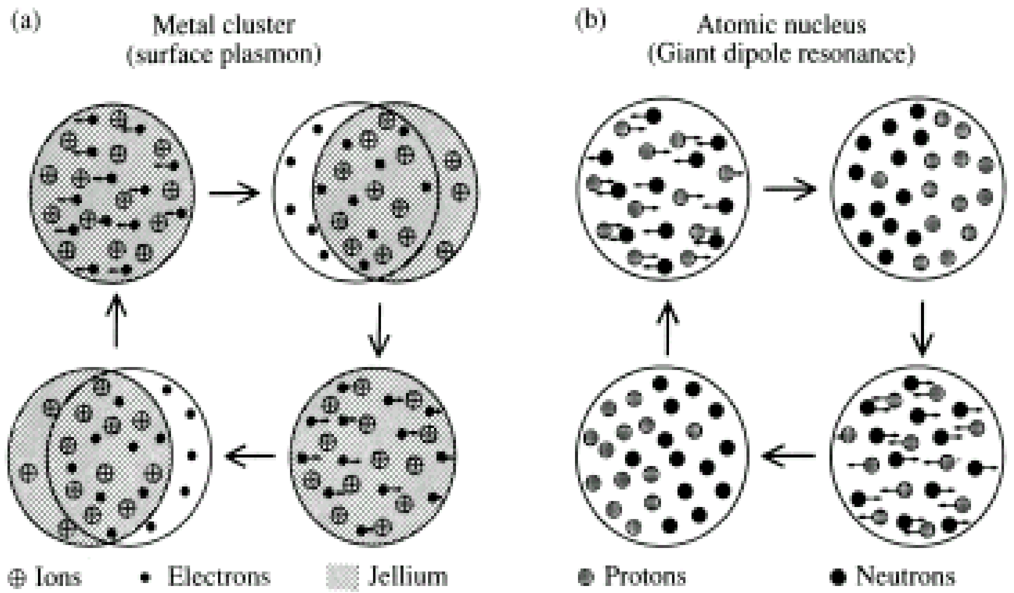
B.A. Li et al., Prog. Part. Nucl. Phys. **99**, 29 (2018)

Symmetry energy from IV vibrations

Neutrons and protons oscillate in opposition of phase.

$$E_{\mathrm{IVGR}} \approx \sqrt{\frac{\partial^2 E}{\partial \beta^2}} \approx \sqrt{S(\rho)}$$

$$\beta \equiv \frac{\rho_n - \rho_p}{\rho}$$



Promising observables to extract the properties of the symmetry energy.

Problems:
the nucleus is not a homogeneous system, it has a shell structure, and there is isoscalar/isovector mixing.

ECT*, 9/7/2025

Giant Quadrupole Resonance

PHYSICAL REVIEW C **88**, 044310 (2013)

Systematics of isovector and isoscalar giant quadrupole resonances in normal and superfluid spherical nuclei

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(Received 9 July 2013; revised manuscript received 13 September 2013; published 11 October 2013)

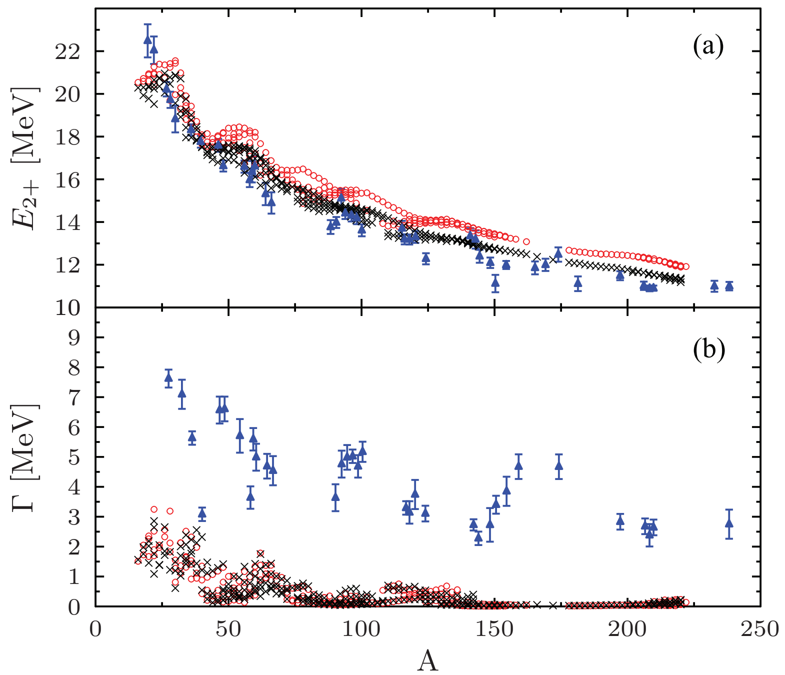

FIG. 9. (Color online) Collective energy (a) and width (b) of the IS GQR systematically obtained for spherical nuclei using the SkM* (black crosses) and Sly4 (red circles) functionals. The blue triangles correspond to experimental data taken from [8].

PHYSICAL REVIEW C **87**, 034301 (2013)

Giant quadrupole resonances in ^{208}Pb, the nuclear symmetry energy, and the neutron skin thickness

X. Roca-Maza,[1,2] M. Brenna,[1,2] B. K. Agrawal,[3] P. F. Bortignon,[1,2] G. Colò,[1,2] Li-Gang Cao,[4] N. Paar,[5] and D. Vretenar[5]
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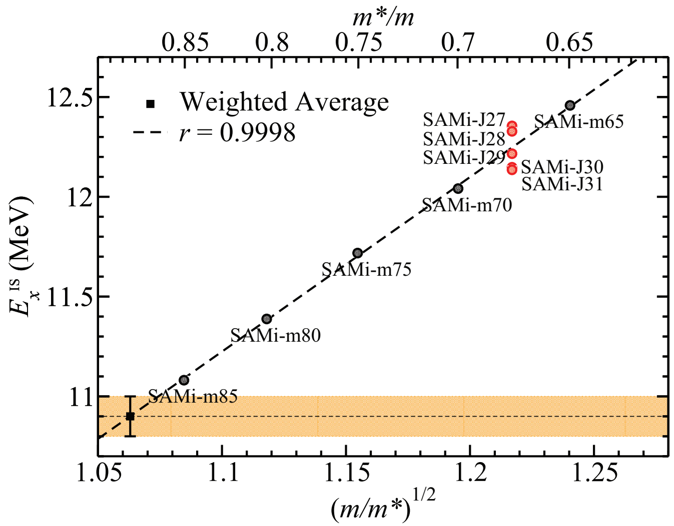
(Received 18 December 2012; published 1 March 2013)



The ISGQR energy is sensitive to the effective mass.

Reminder on effective mass

$$E = \frac{\hbar^2 k^2}{2m} + \Sigma(k, E)$$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} + \frac{d\Sigma}{dE}\frac{dE}{dk} + \frac{d\Sigma}{dk}$$

$$\frac{dE}{dk}\left(1 - \frac{d\Sigma}{dE}\right) = \frac{\hbar^2 k}{m} + \frac{d\Sigma}{dk}$$

If we wish to define

$$E \equiv \frac{\hbar^2 k^2}{2m^*} \rightarrow \frac{dE}{dk} = \frac{\hbar^2 k}{m^*}$$

then

$$\frac{\hbar^2 k}{m^*} = \left(1 - \frac{d\Sigma}{dE}\right)^{-1}\left(\frac{\hbar^2 k}{m} + \frac{d\Sigma}{dk}\right)$$

$$\frac{m}{m^*} = \left(1 - \frac{d\Sigma}{dE}\right)^{-1}\left(1 + \frac{m}{\hbar^2 k}\frac{d\Sigma}{dk}\right)$$

Here, E is the single-particle energy, NOT the total energy.

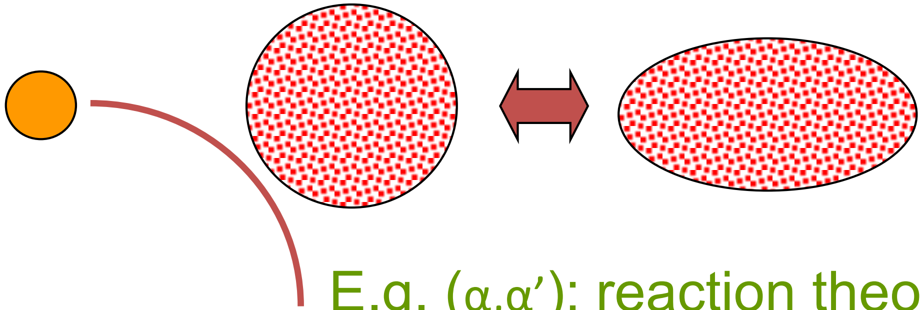
The effective mass, in particular m*/m, is related to the density of s.p. states.

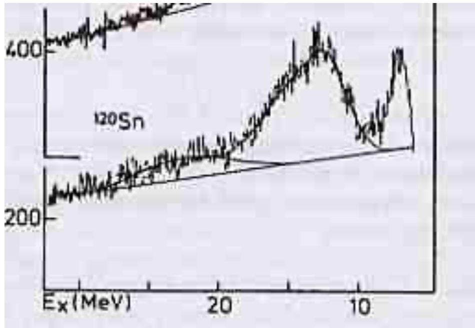
$$m^*/m \approx 0.7 - 1$$

First term: E-mass

Second term: k-mass

GRs excited in inelastic scattering





E.g. (α,α'): reaction theory should be used

DWBA

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \quad f(\theta) = -\frac{m}{2\pi\hbar^2}\int d^3R\ \chi_f^*(R)\langle f|V_{Aa}|i\rangle\chi_i(R)$$

Simplifying (not realistic) assumptions: zero-range force, distorted waves reduced to plane waves:

$$V_{Aa} = \sum_i v_0\delta(\vec{R}-\vec{r}_i)$$

$$e^{i\vec{q}\cdot R} = 4\pi\sum_{LM} i^{-L} j_L(qR) Y^*_{LM}(\hat{q}) Y_{LM}(\hat{R})$$

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int d^3R \; \chi_f^*(R) \langle f | V_{Aa} | i \rangle \chi_i(R)$$

With the previous assumptions:

$$f(\theta) \sim \sum_i \sum_{LM} \langle f | j_L(qr_i) Y_{LM}(\hat{r}_i) | i \rangle Y^*_{LM}(\hat{q})$$

If the argument is small,

$$j_l(qr_i) \sim r_i^L$$

and then the cross section for a given L is proportional to the matrix element of

$$\sum_i r_i^L Y_{LM}(\hat{r}_i)$$